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On Essential Selfadjointness of Dirac Operators

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§1. Introduction. The Hamiltonians in quantum mechanics are postulated to be selfadjoint operators. On the other hand they are given mostly as formal differential expressions. So it occures the question whether these expressions determine selfadjoint operators uniquely or not in a suitable Hilbert space $\mathcal{H}$. For example, the Hamiltonians in relativistic quantum mechanics are given by the Dirac operators:

$$(1.1) \qquad T = -i \sum_{j=1}^{3} \alpha_j \, \partial/\partial x_j + V, \qquad i = \sqrt{-1},$$

where $V = V(x)$ is a 4×4 symmetric matrix and α_j are 4×4 constant symmetric matrices satisfying the anti-commutation relations

$$(1.2) \qquad \alpha_j \alpha_k + \alpha_k \alpha_j = 2 \delta_{jk} I \qquad (j,k = 1,2,3).$$

Now, let $\mathcal{H}$ be the Hilbert space $\mathcal{H} = [L^2(R^3)]^4$ and $\mathcal{D}_o$ be the linear subset $\mathcal{D}_0 = [C_0(R^3\setminus\{0\})]^4$. Let T_0 be the restriction of T on $\mathcal{D}_0$. Then, under each assumption mentioned latter, the range of T_0 is included in $\mathcal{H}$, and the operator T_0 is symmetric in $\mathcal{H}$. Thus our problem becomes: Is the operator T_0 essentially selfadjoint?

§2. results. Many arthers have obtained the affermative results on this problem under some assumptions on the potential V. Their assumptions will be, I think, classified into two groups:

(I) (Coulomb type) $|V| \leq k/|x|$,

where $|V|$ denotes the norm of symmetric matrix V. under this assumption, it holds the inequality

(2.1) $\|Vu\| \leq a\|S_0u\| + b\|u\|, \quad {}^{\forall}u \in \mathcal{D}_o$

with $a = 2k$ and $b = 0$, where S_0 is the operator T_0 with $V = 0$. Thus T_0 is essentially selfadjoint if $k \leq \frac{1}{2}$. This is a result of Kato [7]; see also [8 ;chap.V, §5.4].

(II) (singularity more gentle than the Coulomb type)

(II.1) $|V| \in L^3_{\underline{loc}}$ . . . (Gross [3]).

(II.2) (Stummel type) The function of x

$$\int_{|x-y|\leq 1} |V(x)|^2 \, |x-y|^{-1-\varepsilon} \, dy$$

is <u>locally</u> bounded for some $\varepsilon > 0$. . . . (Evans [2]).

Now, we remark that the inequality (2.1) holds with arbitrary small a under the assumptions (II.1) or (II.2) without the underlined parts; see also Jörgens [5]. This is also true under the next assumption without the underlined parts; see Schechter [11; p.138]:

(II.3) The function of x

$$\int_{|x-y|\leq \delta} |V(x)|^2 \, |x-y|^{-1} \, dy$$

is <u>locally</u> bounded and tends to zero as $\delta \downarrow 0$ uniformly <u>on every compact set</u>.

On the other hand, it holds that

Theorem 1. Let V^R be the potential defined by $V^R(x) = V(x)$ for $|x| \leqq R$ and $V^R(x) = 0$ for $|x| > R$ and T^R_o be T_o with V replaced by V^R. Assume that T^R_o ($\forall R>0$) is essentially selfadjoint and the domain of its unique selfadjoint extension coincides with the domain of S_o^*, which is the Sobolev space $[H^1]^4$. Then T_o is also essentially selfadjoint.

Combining with these results we have

Thereom 2. Let $V = V_1 + V_2 + V_3$, where V_1 satisfies the assumption (I) with $k < \frac{1}{2}$ and V_2 and V_3 satisfy (II.1) and (II.3) (with the underlined parts), respectively. Then, the operator T_o is essentially selfadjoint.

This is essentially a result of Jörgens [5].

Now, let us return to the assumption of type (I). We restrict our attention to the potential V to be a scalar $q(x)$ times the 4×4 unit matrix I;

(I.1) $\quad V(x) = q(x)\, I,$

or to be more restriced one:

(I.2) $\quad q(x) = k/|x|.$

Then, Rellich [10] and Weidmann [14] show that under the assumption (I.2) T_o is essentially selfadjoint if and only if $|k| < \sqrt{3}/2$. The "if part" is extended by Schminke [12], and Gustufson and Rejto [4] under the assumption (I.1), and by Kalf [6] under the assumption [I].

Comparing with these results and Theorem 2, it occures the question whether one can replace the number $\frac{1}{2}$ in Theorem 2 by more grater one or not. I claim that this is negative:

Theorem 3. For any $k > \frac{1}{2}$ there exists a matrix $V(x)$ such that it satisfies (I.1) and the Dirac operator T_0 with this potential V is not essentially selfadjoint.

Although Theorem 1 is similar to a special case (Remark 5.5) of Theorem 5.6 of Jörgens [5], we shall give another proof of it in §3. Our method is based on an idea of Chernoff [1]. In §4 we construct a potential V which has the properties stated in Theorem 3.

§3. Proof of Thoerm 1. Let us consider a solution of the equation

$$du/dt = i\,Tu, \qquad u(0) = u_0 \in [H^1]^4. \tag{3.1}$$

Standard arguments show that

Lemma 1. Let u be a solution of the equation (3.1) in $[H^1([-t_0,t_0] \times R^3)]^4$ and put $D_t = \{ x \in R^3 ; |x-x_0| \leq d-|t| \}$ for $|t| \leq t_0 < d$. Then, we have,

$$\int_{D_{\pm t_0}} |u|^2\, dx \leq \int_{D_0} |u|^2\, dx. \tag{3.2}$$

In particular, if $u_0 = 0$ in D_0, then $u(t) = 0$ in D_t and if $\text{supp}\, u_0 \subset \{x \in R^3;\ |x| < R\}$, then $\text{supp}\, u(t) \subset \{x;\ |x| < R + |t|\}$ for $|t| \leqq t_0$.

Let $\mathcal{D}_1$ be the set of C^4valued functions which are in $[H^1]^4$ and have compact supports.

Lemma 2. Let $u_0 \in \mathcal{D}_1$. Then the equation (3.1) has the unique solution $u(t) \in \mathcal{D}_1$, which satisfies the equality

(3.3) $\|u(t)\| = \|u(0)\|$.

Proof. Let $u_0 \in \mathcal{D}_1$ and $\text{supp}\, u_0 \subset \{x:\ |x| < R/2\}$. Then the equation $du/dt = i\,T^R u$, $u(0) = u_0$ has the unique solution $u(t) \in [H^1]^4$ satisfying (3.3) since $T^R \,|\, [H^1]^4$ is self-adjoint by the assumption of Theorem 1. The derivative du/dt is strong sence so that $u \in [H^1([-t_0, t_0] \times R^3)]^4$ and $\text{supp}\, u(t) \subset \{x;\ |x| < R/2 + |t|\}$ by virtue of Lemma 1. Thus $u(t)$ is a solution of (3.1) for $t < R/2$, which proves the present Lemma since R can be chosen arbitrary large and the uniqueness follows from (3.2).

Proof of Theorem 1. Let $T_1 = T \,|\, \mathcal{D}_1$. Then, it is easy to see that the closure of T_0 = the closure of T_1 so that $T_1{}^* = T_0{}^*$.

Let $\psi_{\pm}$ be solutions of the equations $T_0{}^*\psi_{\pm} = T_1{}^*\psi_{\pm} = \pm i\,\psi_{\pm}$ and $u(t)$ be as above. Put $f_{\pm}(t) = (\,u(t), \psi_{\pm})$. Then, we have $(d/dt)f_{\pm}(t) = ((d/dt)u(t), \psi_{\pm}) = (iT_1{}^*u(t), \psi_{\pm}) = (iu(t), \pm i\,\psi_{\pm}) = \pm\, f(t)$ so that $f_{\pm}(t) = f_{\pm}(0)\, e^{\pm t}$. On the other hand the equality (3.3) implies that $f_{\pm}$ are bounded. Thus we have $f_{\pm}(0) = (\,u_0, \psi_{\pm}) = 0$, which implies $\psi_{\pm} = 0$ since $u_0 \in \mathcal{D}_1$ is arbitrary. Thus we complete the proof.

§4. Proof of Theorem 3. We define, as is done in standard textbooks on quantum mechanics, the constant symmetrix 2×2 matrices σ_j(j=1,2,3) by

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \text{ and } \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

They satisfy the relations

$$\sigma_j\sigma_k = i\,\sigma_l, \quad (j,k,l) = (1,2,3) \text{ in the cyclic order}$$

and the anti-commutation relations

$$\sigma_j\sigma_k + \sigma_k\sigma_j = 2\,\delta_{jk}\,I.$$

(Here and in the sequel, we sometimes denote by I the 2×2 unit matrix and sometimes the 4×4 unit matrix. But no confusion will occur.) Define α_j by $\alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}$. Then, the equality $\alpha_j \alpha_k = \begin{pmatrix} \sigma_j \sigma_k & 0 \\ 0 & \sigma_j \sigma_k \end{pmatrix}$ holds so that α's satisfy the anti-commutation relations (1.2). Put $\sigma_r = \sum_{j=1}^{3} \sigma_j x_j / r$ and $\alpha_r = \sum_{j=1}^{3} \alpha_j x_j / r$, $r = |x|$. Then, the anti-commutation relations yield $\sigma_r^2 = I$ and $\alpha_r^2 = I$. Put $J = \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix}$ and $U = \begin{bmatrix} I & 0 \\ 0 & i\sigma_r \end{bmatrix}$. Then, it holds that

$$(4.1) \qquad U \alpha_r = i J U.$$

Define σ_j' by $\sigma_j' = \begin{pmatrix} \sigma_j & 0 \\ 0 & \sigma_j \end{pmatrix}$ and the differential operators M_j by $M_j = x_k \partial/\partial x_l - x_l \partial/\partial x_k$, where $(j,k,l) = (1,2,3)$ in the cyclic order. Then, we have

$$(4.2) \qquad \begin{aligned} \sum_j \alpha_j \partial/\partial x_j &= \alpha_r^2 \Big(\sum_j \alpha_j \partial/\partial x_j \Big) = \\ &= \alpha_r \Big(\sum_j \alpha_j^2 r^{-1} x_j \, \partial/\partial x_j + \sum_{j \neq k} \alpha_j \alpha_k r^{-1} x_j \, \partial/\partial x_j \Big) \\ &= \alpha_r \Big(\partial/\partial r + i\, r^{-1} \alpha_r \sum_j \sigma_j' M_j \Big). \end{aligned}$$

Now, let u be a solution of the equation

$$(4.3) \qquad T u = -i \sum_j \alpha_j \partial/\partial x_j \, u + V u = \lambda u$$

and assume that $w = Uu$ depends only upon r. Multiplication from the left by U yields

$$(4.4) \qquad JU(\partial/\partial r)U^{-1} w + i r^{-1} J \begin{bmatrix} 0 & 0 \\ 0 & -2iI \end{bmatrix} w + UVU^{-1} w = \lambda w,$$

using (4.1),(4.2) and the identity $U(\sum_j \sigma_j' M_j)u = \begin{pmatrix} 0 & 0 \\ 0 & -2iI \end{pmatrix} w$.

Let the potential V be

$$(4.5) \qquad V(x) = r^{-1} \begin{pmatrix} aI & ib\,\sigma_r \\ -ib\,\sigma_r & aI \end{pmatrix}.$$

Then, $UVU^{-1} = r^{-1} \begin{pmatrix} aI & bI \\ bI & aI \end{pmatrix}$, so that the eigenvalues of V are $(a \pm b)/r$. Assume moreovere that

$$w = r^{-1}\ {}^t(\ f(r), f(r), g(r), g(r)\ ).$$

Then, the equality (4.4) reduces to

$$(4.6) \quad \begin{cases} f' - r^{-1}f + r^{-1}(bf + ag) = \lambda g \\ -g' - r^{-1}g + r^{-1}(af+bg) = \lambda f. \end{cases}$$

As to this system of differential equations, as is pointed out by Weidmann [14], analogie to the Weyl's alternative theorem on Strum-Liouville equations holds;

Lemma 3. (i) If every pair $\{f,g\}$ of solutions of (4.6) satisfy

$$(4.7) \qquad \int_0^1 |f|^2 + |g|^2\, dr < +\infty$$

for some $\lambda = \lambda_0$, then every pair of solution of (4.6) also have the property (4.7) for arbitrary $\lambda \in C$.

(ii) For every non-real λ, the system (4.6) has at least one non-trivial solution which has the property (4.7).

The above assertions (i) and (ii) are also valid when the inequality (4.7) is replaced by

(4.7)' $\displaystyle\int_1^{\infty} |f|^2 + |g|^2 \, dr < +\infty.$

Let $|b-1| \neq |a|$. Then, the system (4.6) with $\lambda = 0$ has a fundamental system $\{f_{\pm}, g_{\pm}\} = r^{\rho_{\pm}}\{1, (1-b-\rho_{\pm})/a\}$ of solutions, where $\rho_{\pm} = \pm\sqrt{(b-1)^2-a^2}$. The both pairs $\{f_{\pm}, g_{\pm}\}$ satisfy (4.7) if and only if $(b-1)^2-a^2 < \frac{1}{4}$, and then both pairs have not the property (4.7)'.Thus Lemma 3 shows that if

(4.8) $\qquad \frac{1}{4} > (b-1)^2-a^2 \neq 0,$

then the system (4.6) with non-real λ has non-trivial pair $\{f, g\}$ of solution satisfying $\int_0^{\infty} |f|^2 + |g|^2 \, dr < +\infty$. Then, u is a non-trivial solution of (4.3) belonging to $\mathcal{H}$ since $\|u\|^2 = \|w\|^2 = 8\int_0^{\infty} |f|^2 + |g|^2 \, dr < +\infty$. The definition of the adjoint operators and integration by parts show that $u \in \mathcal{D}(T_0^*)$ and $T_0^* u = \lambda u$. Thus T_0 is not essentially selfadjoint since λ is non-real. Let, for example, $b = \frac{1}{2}$ and $a > 0$. Then, $|V(x)| = (\frac{1}{2}+a)/r$ and the condition (4.8) is satisfied for $a \neq \frac{1}{2}$.

Last, we remark that the operator T_0 with V defined by (4.5) has a selfadjoint extension. Indeed, let $\tilde{J}$ be the antilinear operator defined by $\tilde{J}u = \sigma_2' \, \bar{u}$, then T_0 commutes with $\tilde{J}$ so that T_0 is $\tilde{J}$-real.

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